Optimal Design Construction With Constraints I.

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Abstract:

This is an attempt to survey various approaches developed in experimental design when some constraints are imposed. These constraints are on the total cost of experiment, the location of supporting points, value of the auxiliary objective functions, and so on. The basic idea of the survey is that all corresponding optimization problems can be imbedded in the convex theory of experimental design. Part I. is concerned with the properties of optimal designs, while Part II. will be devoted mainly to numerical methods.

I. Introduction

Experimental design problems considered in this paper are basically related to the standard linear regression model:

$$y_{ij} = \theta^T f(x_i) + \varepsilon_{ij}, \qquad (1)$$
$$i=1,\dots,n, \quad j=1,\dots,r_i, \quad \Sigma\, r_i=N,$$

where $\theta \in R^m$ are unknown parameters, $f^T(x) = (f_1(x),\dots,f_m(x))$ are given functions, supporting points x can be chosen from some set X, ε_{ij} are uncorrelated random errors with zero means and variances equal to 1.

For the best linear unbiased estimator of unknown parameters the accumulated "accuracy" is described by the information matrix:

$$M(\xi) = N^{-1}\Sigma\, p_i f(x_i) f^T(x_i), \quad p_i = r_i/N,$$

which is completely defined by design $\xi = \{x_i, p_i\}_1^N$. In the context of the convex design theory:

$$M(\xi) = \int f(x) f^T(x) \xi(dx),$$

where $\xi(dx)$ is a probability measure or (continuous) design with the supporting set belonging to X : *supp* $\xi \subset X$. The subscript corresponding to the area of integration will be used only when it will be essential for understanding. A design

$$\xi^* = \operatorname*{Arg\,min}_{\xi} \Psi[M(\xi)] \qquad (2)$$

is called (Ψ–)optimal.

In the traditional case minimization has to be over the set of all possible probability measures Ξ with supporting sets belonging to X. For a practitioner it means that one has to find an optimal design with a given number of observations, see (1). Of course, the reality can be worse and more constraints can be imposed. For instance, the cost of observations may depend upon x with the total cost of the experiment not exceeding some level. Sometimes together with the parameters of model (1) one may wish to estimate the parameters of some competing model. Then additionally to (2) it is reasonable to demand that the corresponding information matrix is not very "small". In the observation network optimization problem it is usually not reasonable to locate several sensors at the same site nor with very small distances between them. This leads to the restriction of the number of sensors per square unit. In terms of continuous designs it means that the density of the design measure has to be restricted.

Thus additionally to (2) one has to consider design problems when the structure of Ξ is more complicated than in the traditional experimental design theory, which is very briefly surveyed in Section II. In Sections III–V the various types of constraints are considered, and the main focusing is on the similarities among the corresponding results rather than on the discrepancies between them.

II. Standard Equivalence Theorem

The optimization problem (2) has been intensively studied since Kiefer's pioneering paper (1959). In this section we shall summarize the major properties of the traditional optimal designs.

Assume that:

(a) X is compact;

(b) f(x) are continuous functions in X, $f \in R^m$;

(c) $\Psi(M)$ is a convex function;

(d) there exists q such that

$$\{\xi : \Psi[M(\xi)] \leq q < \infty\} = \Xi(q) \neq \emptyset;$$

(e) for any $\xi \in \Xi(q)$ and $\bar{\xi} \in \Xi$:

$$\Psi[(1-\alpha)M(\xi)+\alpha M(\bar{\xi})] = \Psi[M(\xi)] + \alpha\int\psi(x,\xi)\bar{\xi}(dx) + \tau(\alpha,\xi,\bar{\xi}),$$

where $\tau(\alpha,\xi,\bar{\xi})=o(\alpha)$.

Assumptions (c) and (e) are most essential and restrictive for the theory. Fortunately the majority of the popular optimality criteria satisfy them, such as D– and linear criteria with regular optimal designs. But there exist some natural and widely used criteria which do not satisfy (e) (for instance, the minimax ones). One can face similar troubles even for "good" criteria when an optimal design happens to be singular; see Silvey (1980), Pukelsheim (1980).

Theorem 1. If (a)–(e) hold, then:

1. For any optimal design there exists a design with the same information matrix and containing no more than $n = m(m+1)/2$ supporting points.

2. A necessary and sufficient condition for a design ξ^* to be optimal is fulfillment of the inequality

$$\min_{x\in X} \psi(x,\xi^*) \geq 0. \tag{3}$$

3. The set of optimal designs is convex.

4. $\psi(x,\xi^*)$ achieves zero almost everywhere in *supp* ξ^* .

Proof. The proof of this theorem is well known and belongs to the rim of textbooks, and is only sketched here to clarify the main ideas which are used in the subsequent sections. The proof of the first part of the theorem is based on Caratheodory's theorem and on the fact that any information matrix can be considered as an element of the convex hull of the elementary informationmatrices:

$$m(x) = f(x)f^T(x) \in R^{m(m+1)/2},\ x \in X.$$

Necessity and sufficiency of (3) follows from the fact that the following inequality:

$$\min_{\xi\in\Xi} \lim_{\alpha\to o} \psi[(1-\alpha)M(\xi^*) + \alpha M(\xi)] \geq 0 \tag{4}$$

is a necessary and sufficient condition of optimality of ξ^*. If (e) holds, then (4) can be easily transformed to:

$$\min_{\xi\in\Xi} \int\psi(x,\xi^*)\xi(dx) = \min_{x\in X} \psi(x,\xi) \geq 0.$$

The third part of the theorem follows directly from the convexity of the objective function.

Integration of both parts of the expression from (e) with respect to $\xi^*(dx)$ confirms the final section of the theorem.

Theorem 1 is the basic one in convex design theory and its various modifications have been extensively discussed in the statistical literature: see Fedorov (1972), Fedorov and Malyutov (1972), Whittle (1973), Silvey (1980).

Example 1. For the D–criterion, when $\Psi(M) = -\ln|M|$ and

$$\psi(x,\xi) = m - d(x,\xi),\ d(x,\xi) = f(x)^T M^{-1}(\xi)f(x)\ ,$$

Point 2 of the theorem can be reformulated in the more traditional form:

The following problems:

$$\xi^* = \operatorname{Arg}\max_{\xi} \ln|M(\xi)|;$$

$$\xi^* = \operatorname{Arg}\min_{\xi}\max_{x\in X} d(x,\xi);$$

$$\max_{x\in X} d(x,\xi) = m;$$

are equivalent.

This is Kiefer's celebrated equivalence theorem.

III. Linear Constraints

Constraints linear with the respect to the design measure mainly arise in experiments when the cost of observations depends upon controlled variables. The optimization problem can be stated now in the following way:

$$\xi^* = \operatorname{Arg}\min_{\xi} \Psi[M(\xi)] \tag{5}$$

$$\text{s.t.} \int\xi(dx) = 1, \quad C(\xi) = \int\phi(x)\xi(dx) \leq 0, \tag{6}$$

where $\phi(x) = (\phi_1(x),...,\phi_l(x))^T$.

Example 2. Let the functions $\zeta_\alpha(x)$, $\alpha=1,...,l$, describe the losses when observation is taken at point x. Assume that the total loss for a particular α can not exceed C_α. Then

$$\Sigma\, r_i \zeta_\alpha(x_i) \le C_\alpha, \qquad \alpha = 1,...,l,$$

where r_i is the number of observations at point x_i.

For continuous designs the latter inequality takes the form:

$$\int \phi(x)\xi(dx) \le 0,$$

where $\phi_\alpha(x) = \zeta_\alpha(x) - c_\alpha$, $c_\alpha = C_\alpha/N$.

We consider the optimization problem (6) under assumptions (a)–(e) adding to them (b') $\phi(x)$ are continuous for all $x \in X$.

Theorem 2. If (a)–(e),(b') hold, then

1. For any optimal design there exists a design with the same information matrix and containing no more than $n_0 = m(m+1)/2 + l$ supporting points.
2. A necessary and sufficient condition for a design ξ^* to be optimal is fulfillment of the inequality

$$\min_x \; q(x,u^*\xi^*) \ge 0,$$

where

$$q(x,u,\xi) = \psi(x,\xi) + u^T\phi(x),$$

$$u^* = \operatorname{Arg}\max_{u \in U'} \min_{x \in X} q(x,u,\xi^*),$$

$$U' = \{u: u \in R^l,\, u_\alpha \ge 0\}.$$

3. The set of optimal designs is convex.

4. $q(x,u^*,\xi^*)$ achieves zero almost everywhere in *supp* ξ^*.

Proof. To prove the first part of the theorem it is sufficient to notice that any couple $\{M(\xi),C(\xi)\}$ belongs to the convex hull of

$$\{m(x),\, \phi(x)\} \in R^{m(m+1)/2+l},\ x \in X.$$

and then to apply to Caratheodory's theorem.

To prove the second part of the theorem one has to add to (4) the constraints (6):

$$\min_{\xi \in \Xi} \int \psi(x,\xi^*)\xi(dx), \qquad (7)$$

$$\text{s.t.} \quad \int \phi(x)\xi(dx) \le 0. \qquad (8)$$

The fulfillment of (7) and (8) are necessary and sufficient condition for the optimality of ξ^*. But unlike the standard case there is generally no single point design (see comments to (4)) simultaneously satisfying (7) and (8).

The Lagrangian technique (see, for instance, Laurent (1972), Ch. 7) leads to the duality of optimization problem from (7), (8) with the following maximin problem:

$$\max_{u \in U'} \min_{\xi} \int q(x,u,\xi^*)\xi(dx),$$

or equivalently

$$\max_{u \in U'} \min_{x \in X} q(x,u,\xi^*)$$

(see, for instance, Fedorov and Gaivoronski (1984)) confirming the assertion of the theorem. The proof of two last parts of the theorem is identical to the standard case

Note 1. The existence of a solution of (7), (8) with no more than $(l+1)$ supporting points follows from Caratheodory's theorem .

Note 2. In the frame of Example 2 constraints (6) means that one is constrainted both in the number of observations:

$$\sum_{i=1}^{n} r_i = N \quad \Rightarrow \quad \int \zeta(dx) = 1$$

and in their total cost $(l = 1)$:

$$\sum_{i=1}^{n} r_i \ \zeta(x_i) \le C \quad \Rightarrow \quad \int \phi(x)\ \xi\ (dx) \le 0 \ \text{ or} \int \zeta\ (x)\ \xi\ (dx) \le c.$$

It is essential that there are two linear constraints. If one refuses the first one (total number of observations is given), then the transformation

$$\xi'(dx) = \phi(x)\ \xi\ (dx), \quad f'(x) = \phi^{-1/2}\ (x)\ f(x)$$

returns us to the standard case, see (2). Compare with Chernoff (1972 p. 16) and Fedorov (1972 p. 59).

Example 3. Let us consider the design problem for one dimension polynomial response and D–criterion:

$$f_\alpha(x) = x^{\alpha-1},\ |x| \le 1,\ \Psi(M) = -\ln|M|,$$

with linear constraints:

$$\int_{-1}^{1} \phi(x)\xi(dx) \le 0,$$

and let $\{f,\phi\}$ constitute a Chebyshev system on $|x|\le 1$.
From example 1 it follows that

$$q(x,u,\xi) = m - \Sigma\, M_{\alpha\beta}^{-1} x^{\alpha-1} x^{\beta-1} + u^{T}\phi(x),$$

i.e. $q(x,u,\xi)$ is a linear combination of $2m+l$ Chebyshev's functions with some nonzero coefficients. Therefore (see, for instance, Karlin and Studden (1966)) this function has no more than $2m+l$ roots and subsequently has no more than $m+l/2$ (if l is even) or $m+(l+1)/2$ (if l is odd) minimal on the interval $|x|\le 1$. But in accordance with Theorem 2 they have to coincide with the support points. So for this case the number of support points is essentially less than n_0.

IV. Nonlinear Convex Constraints

The approach considered in the previous section can be used for the more general design problem:

$$\xi^* = \operatorname*{Arg\,min}_{\xi} \Psi[M(\xi)], \tag{9}$$

$$\text{s. t.} \quad \Phi(\xi) \le 0,\ \ \Phi \in R^{l}. \tag{10}$$

Assume additionally to (a)–(e),(b') that:
(c') $\Phi(x)$ are convex;
(e') $\Phi[(1-\alpha)\xi + \alpha\bar{\xi}] = \Phi(\xi) + \alpha\int\phi(x,\xi)\bar{\xi}(dx) + \tau(\alpha,\xi,\bar{\xi})$, where $\tau_k(\alpha,\xi,\bar{\xi}) = o(\alpha)$, $k = 1,\ldots,l$, ξ and $\bar{\xi}$ are defined in (e) with $\Xi(q)$ and Ξ satisfying (10).

The analysis of (9),(10) are mainly based on ideas of Theorem 2 and on the possibility of linearization of $\Phi(\xi)$ near an optimal design (compare with Gaivoronski (1984) and Lee (1988)).

All the final results can be described by Theorem 2 with functions $\phi(x,\xi)$ defined in (e') and $\Phi(\xi) = 0$. Of course, it is assumed that the set of ξ satisfying (1) is not empty and all constraints are active. We shall refer to Theorem 2' in the case of nonlinear constraints, but one has to remember about assumptions (c'),(e').

Example 4. Let $\Psi = -\ln|M|$ and $\Phi_k = -\ln|M| - c_k$, where

$$M_k(\xi) = \int f_k(x) f^T_k(x)\xi(dx).$$

Then the design problem corresponds to the case when one wishes to find a D–optimal design for the response $\theta^T f(x)$ and to be sure that thi design is efficient for some competing responses $\theta^T_k f_k(x)$. Taking into account that:

$$\psi(x,\xi) = m - d(x,\xi),$$

$$\phi_k(x,\xi) = m_k - d_k(x,\xi),$$

$$d_k(x,\xi) = f^T_k(x) M^{-1}_k(\xi) f_k(x),$$

and assuming that $f(x)$ and $f_k(x)$, $k=1,\ldots,l$ are continuous in X and c_k are not very small (to provide fulfillment of (d) together with (10)) it is not difficult to check the validity of Theorem 2'. From this theorem it follows that:

a necessary and sufficient condition for optimality of ξ^* is existence of $u^* \in U'$such that

$$d(x,\xi^*) + \Sigma\, u^*_k d_k(x,\xi^*) \le m + \Sigma\, u^*_k m_k$$

while $\Phi(\xi) = 0$;
almost everywhere in *supp* ξ^*

$$d(x,\xi^*) + \Sigma\, u^*_k d_k(x,\xi^*) = m + \Sigma\, u^*_k m_k.$$

A number of similar examples for various optimality criteria can be found in Lee (1988).

Theorems 1 – 2' can be considered as specific cases of the Kuhn–Tucker Theorem, and, of course, its versions and generalizations of this theorem can help to extend the previous results.

For instance, the Kuhn–Tucker Theorem for the case with a continuum of constraints (see Pshenichnyi (1969), Ch. 5.2) allows analysis of the following design problems:

$$\xi^* = \operatorname*{Arg\,min}_{\xi} \Psi[M(\xi)], \tag{11}$$

$$\text{s. t. } \Phi(\xi,\lambda) \le 0,\ \ \Phi \in R^l,\ \ \lambda \in \Lambda \subset R^1. \tag{12}$$

Let there be in addition to the previous assumptions:
(c") $\Phi(\xi,\lambda)$ is convex for all $\lambda \in \Lambda$ and Λ is compact;
(e") $\Phi[(1-\alpha)\xi + \alpha\bar{\xi},\ \lambda] = \Phi(\xi,\lambda) + \alpha \int \phi(x,\xi,\lambda)\bar{\xi}(dx) + \tau(\alpha,\xi,\bar{\xi},\lambda)$, where $\tau(\alpha,\xi,\bar{\xi},\lambda) = o(\alpha)$. Then the above mentioned theorem leads to

Theorem 3. A necessary and sufficient condition for a design ξ^* to be optimal is the existence of such $u^* \in U'$ and $\lambda_k^* \in \Lambda$ that :

$$\min_{x \in X} q(x,u^*,\xi^*) \geq 0, \tag{13}$$

where $q(x,u,\xi) = \psi(x,\xi) + u^T\phi(x,\xi)$, $\Phi(\xi^*,\lambda^*) = 0$,

$\phi_k(x,\xi) = \phi(x,\xi,\lambda_k^*)$, $U' = \{u: u \in R^{l+1}, u_k \geq 0\}$, $k = 1,...,l+1$.

Assume that all λ_k^* are known. Then Theorem 3 states that (11), (12) are equivalent to (9), (10) with $\Phi(\xi)=(\Phi(\xi,\lambda_1^*),..., \Phi(\xi,\lambda^*_{l+1}))^T$. This makes it evident how to use the results of the previous theorems.

Example 5. As in example 4 suppose one wishes to find a D–optimal design for the response $\theta^T f(x)$ and to be sure that this design is efficient for some competing nonlinear response $\eta(x,\lambda)$, i. e.

$$-\ln|M(\xi,\lambda)| \leq c,$$

$$M(\xi,\lambda) = \int f(x,\lambda)f^T(x,\lambda)\xi(dx),\ f(x,\lambda) = \partial\eta(x,\lambda)/\partial\lambda,\ \lambda \in \Lambda \subset R^1.$$

The combination of the results of example 4 and Theorem 3 transforms (13) to:

$$d(x,\xi^*) + \Sigma\, u^*_k d_k(x,\xi^*) \leq m + l\, \Sigma\, u^*_k,$$

$$d_k(x,\xi) = f^T(x,\lambda^*_k)M^{-1}(\xi,\lambda^*_k)f(x,\lambda^*_k),\ k = 1,...,l+1,$$

where

$$\lambda^*_k \in \{\lambda: -\ln|M(\xi^*,\lambda)| = c\}$$

If $f(x)=f(x,\lambda')$, where λ' is a prior value of the parameters λ, this example can be considered as a particular case of the design problem for the nonlinear response, see Atkinson & Fedorov (1988).

V. Directly Constrained Design Measures

A number of experimental design problems can be formulated as optimization problems with explicitly bounded measures (see Fedorov (1986), (1989), Wynn (1982)):

$$\xi^* = \operatorname{Arg} \min_{\xi} \Psi[M(\xi)], \tag{14}$$

$$\text{s. t.} \quad \xi(dx) \leq \Phi(dx),\ \int_X \Phi(dx) = C \geq 1. \tag{15}$$

As in to the moment space theory (see Fedorov (1989), Karlin and Studden (1966), Krein and Nudelman (1973)) ξ^* can be called a Ψ,Φ–optimal design. Assume additionally to (a)–(e) that:

$$\text{(f) } \Phi(dx) \text{ is atomless, i.e. } \lim_{\Delta X \to 0} \int_{\Delta X} \Phi(dx) = 0.$$

Sets Ξ and $\Xi(q)$ in (e) have to satisfy (15).

Let $\bar{\Xi}$ be a set of design measures such that $\xi(\Delta x) = \Phi(\Delta x)$ for any $\Delta X \subset X$. A function $\phi(x,\xi)$ is said to separate sets X_1 and X_2 with respect to the measure $\Phi(dx)$ if for any two sets $\Delta X_1 \in X_1$ and $\Delta X_2 \in X_2$ with equal nonzero measures:

$$\int_{\Delta X_1} \phi(x,\xi)\Phi(dx) \le \int_{\Delta X_2} \phi(x,\xi)\Phi(dx) \ . \tag{16}$$

Theorem 4. If assumptions (a)–(f) hold, then:

1. $\xi^* \in \Xi$ exists.
2. A necessary and sufficient condition of Ψ,Φ–optimality of $\xi^* \in \Xi$ is that $\phi(x,\xi^*)$ separates $X^* = \mathit{supp}\, \xi^*$ and $X \backslash X^*$.

Proof. The results of the theorem are strongly related to the moment spaces theory, and the proof is based on the corresponding ideas.

The existence of an optimal design follows from the compactness of the set of information matrices. The compactness of the latter is provided by (a), (b) and (f). The fact that at least one optimal design belongs to $\bar{\Xi}$ is the corollary of Liapunov's Theorem on the range of a vector measure (see Karlin and Studden, 1966, Ch. VIII).

Necessity follows from the fact that if there exist $\Delta X_1 \subset \mathit{supp}\, X^*$ and $\Delta X_2 \subset X \backslash X^*$ with equal nonzero measures such that:

$$\int_{\Delta X_1} \psi(x,\xi^*)\Phi(dx) > \int_{\Delta X_2} \psi(x,\xi^*)\Phi(dx),$$

then deletion of the first set from the supporting set with the subsequent inclusion of the second one causes the decrease of Ψ. This contradicts the optimality of ξ^*.

Now assume that $\xi^* \in \bar{\Xi}$ is nonoptimal and $\xi \in \bar{\Xi}$ is optimal, i.e.:

$$\Psi[M(\xi^*)] > \Psi[M(\xi)] + \delta, \qquad \delta > 0.$$

Let $\bar{\xi} = (1-\alpha)\xi^* + \alpha\xi$, then:

$$\Psi[M(\bar{\xi})] \le (1-\alpha)\Psi[M(\xi^*)] + \alpha\Psi[M(\xi)]$$

$$< (1-\alpha)\Psi[M(\xi^*)] + \alpha\{\Psi[M(\xi^*)] - \delta\} = \Psi[M(\xi)^*] - \alpha\delta. \tag{17}$$

Simultaneously:

$$\Psi[M(\bar{\xi})] = \Psi[M(\xi^*)] + \alpha \int_X \psi(x,\xi^*)\xi(dx) + o(\alpha)$$

Let $\quad supp\, \xi = (X^* \backslash D) \cup E,\ \ \Delta \subset X^*, E \subset (X \backslash X^*),\ E \cap D = \emptyset$

Then

$$\int_E \Phi(dx) = \int_D \Phi(dx)$$

and

$$\int_X \psi(x,\xi^*)\, \xi(dx) = \int_{X^*} \psi(x,\xi^*)\, \Phi(dx)$$

$$+ \int_E \psi(x,\xi^*)\, \Phi(dx) - \int_D \psi(x,\xi^*)\, \Phi(dx).$$

From assumption (e) it follows that

$$\int_{X^*} \psi(x,\xi^*)\, \Phi(dx) = \int_X \psi(x,\xi^*)\, \xi^*(dx) = 0,$$

and from the statement of the theorem it follows that

$$\min_{x \in E}\ \psi(x,\xi^*) \geq \max_{x \in D}\ \psi(x,\xi^*).$$

Therefore

$$\int_X \psi(x,\xi^*)\, \xi(dx) \geq 0$$

Subsequently

$$\Psi\, [M(\bar{\xi})] \geq \Psi\, [M(\xi^*)] + o(\alpha)$$

The comparison of (17) and (18) gives a contradiction, and this completes the proof.

Note 3. The comparison of Theorems 1 and 4 gives a hint how the latter one can be generalized when to constraints (15) one adds (6), or (10), or (12). For this purpose the function $\psi(x,\xi)$ has to be replaced by a corresponding function $q(x,u,\xi) = \psi(x,\xi) + u^T\phi(x,\xi)$.

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